

RETRIEVAL STUDIES WITH LIDORT

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Final Report
For the period 1 July 2002 through 30 June 2003

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Final Report Summary: NAG5-12317

Retrieval Studies with LIDORT

- (1) NO₂ feasibility from multi-axis ground instruments
- (2) Rotational Raman filling at SBUV wavelengths
- (3) O₃ profile weighting functions in optically thick clouds

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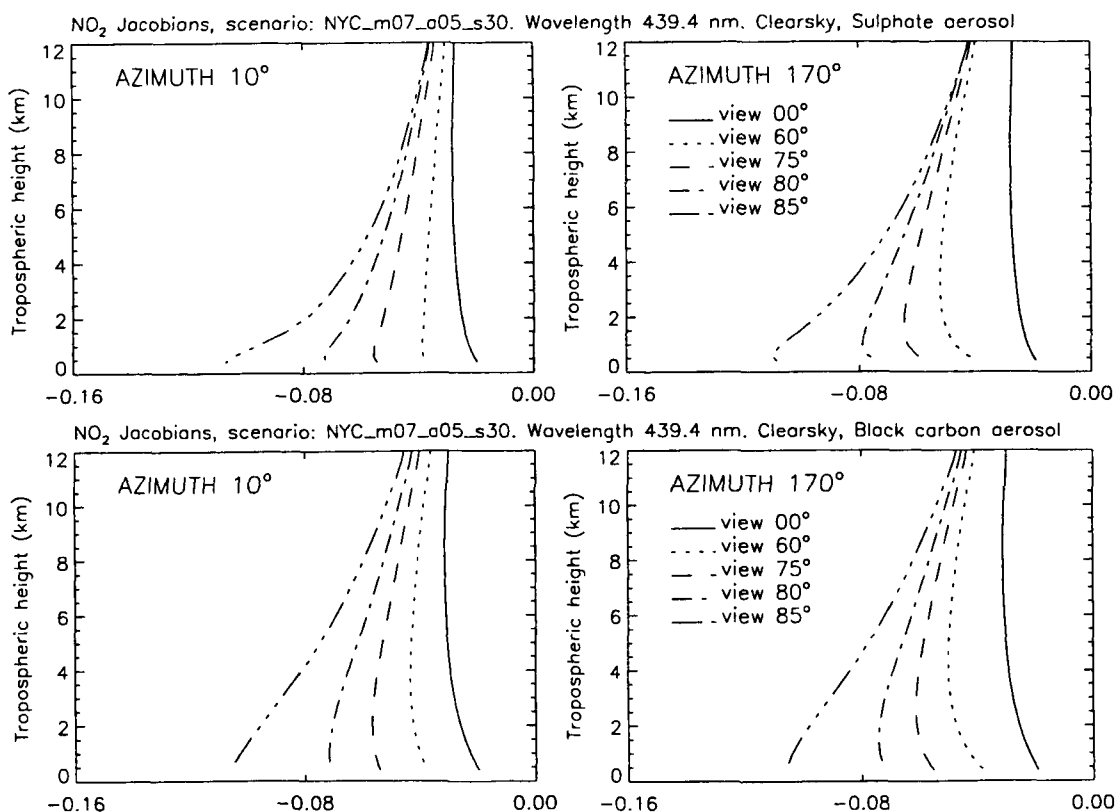
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Abstract

This short program of LIDORT-based research in atmospheric trace gas retrieval was conducted over the 1 year period 01 July 2002 to 30 June 2003. After consultation with the NASA reporting officer, the first of the two original proposal activities (development of a direct-fitting total O₃ column retrieval algorithm with operational capability for GOME data) was replaced by other tasks. The three activities addressed were: (1) Sensitivity studies for column and profile retrieval of NO₂ distributions from a new generation of multi-axis ground-based spectrometers; (2) use of the LIDORT-RRS model to determine the effect of inelastic rotational Raman scattering at SBUV wavelengths; (3) an examination of ozone profile weighting functions in the presence of optically thick tropospheric clouds.

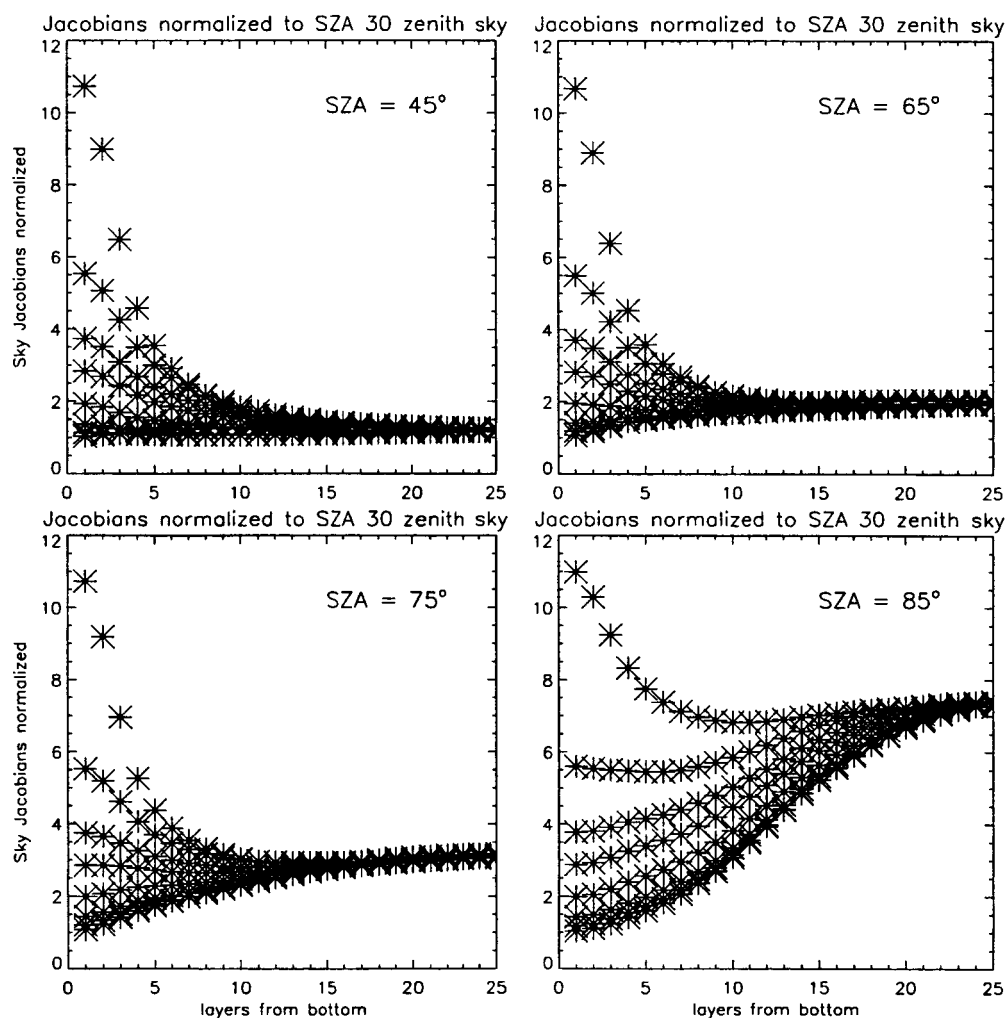
1 Report Summary Task 1

The background for the first task reported here concerns the development of “proof-of-concept” column and profile retrieval algorithms for new ground based multi-axis UV-visible “MAXDOAS” spectrometers with moderate spectral resolution and a multi-angle measurement capability that allows simultaneous spectra to be taken for a range of sky spectra viewing angles. Such instruments are well-suited to ground-based studies aimed at the validation of coincident satellite data, and NASA has become interested in them in the context of a forthcoming NRA for AURA validation. In this report, we focus on the retrieval of profiles of NO_2 from sky spectra in the visible. The LIDORT RT model is well suited to global fitting of a multi-angle sequence of spectra. One call to LIDORT for each wavelength will not only deliver all radiances for the desired range of scan angles, but also all relevant Jacobians both for NO_2 profile distributions and for other model parameter variables (such as aerosol amounts) that will affect retrieval accuracy but are not primary targets of the fit.



In this study, LIDORT Version 2.3 was used to generate analytic NO_2 profile weighting functions for the ground-based downwelling radiation field, for a MAXDOAS-type instrument measuring in the visible; 4 wavelengths in the range 412–450 were selected. Results were obtained for a number of solar zenith angles up to 85°, for 5 viewing angles (0°, 60°, 70°, 80° and 85°) and for relative azimuths

10° and 170° close to the solar and anti-solar planes respectively. A 48-layer atmosphere was used; for the 14 closely-spaced tropospheric layers below about 12 km, pressures and NO₂ volume mixing ratios were taken directly from chemical-model output (GEOSCHEM data for July 1997, as provided by Randall Martin); remaining data was taken from USA AFGL standard atmosphere profiles for pressure, height, temperature and NO₂ and O₃ VMR profiles. Two GEOSCHEM NO₂ mid-latitude profiles were considered (rural and urban pollution scenarios).



Aerosols are an important source of uncertainty in this kind of ground-based retrieval, and the study investigated 6 types of tropospheric and boundary layer aerosols. Profiles are taken from a 1997 run of NASA's aerosol GOCART model, for the sulfate, mineral dust, black carbon, organic carbon, accumulation mode sea-salt, and coarse mode sea-salt types. The example in Figure 1 shows weighting functions at 439.4 nm for layers up to 12 km, for the two reported azimuths, for solar angle 30°, and for 5 lines of sight as indicated. The multi-axis profile sensitivity is evident for both aerosol types shown, but there is greater sensitivity above the lowest layer for the highly absorbing black carbon

aerosol type.

A compilation of results has shown that Jacobians in the lowest layers are insensitive to solar zenith angle. This is illustrated in Figure 2, where Jacobians for a typical run are normalized to their values at SZA 30° . Surface albedo is also seen to have little effect on the sensitivity (in contrast to the situation with remote sensing from space). In the context of this study, other Jacobian runs were performed for both NO_2 and O_3 profiles at UV wavelengths 340 nm and 360 nm. In addition the LIDORT-RRS model (with first-order inelastic rotational Raman scattering - see next section) was used to establish visible wavelengths in the range 400-450 nm at which solar Fraunhofer filling might be an issue for spectral fitting of NO_2 .

Altitude-dependent Air Mass Factors (defined as the derivative of the logarithm of the backscatter with respect to profile, and easily obtainable from the LIDORT radiance and Jacobian output) are a useful indicator of profile sensitivity. Relative AMFs for various elevations were obtained by normalizing against zenith AMFs; for layers above 5 km, these quantities show little variation with elevation. Using these values to generate slant column measurements and assuming 1% variability, one can derive averaging kernels and estimate the degrees-of-freedom-for-signal (trace of the averaging kernel matrix). Initial results indicate that for polluted NO_2 scenarios, 3 good pieces of information can be obtained about the profile below 5 km.

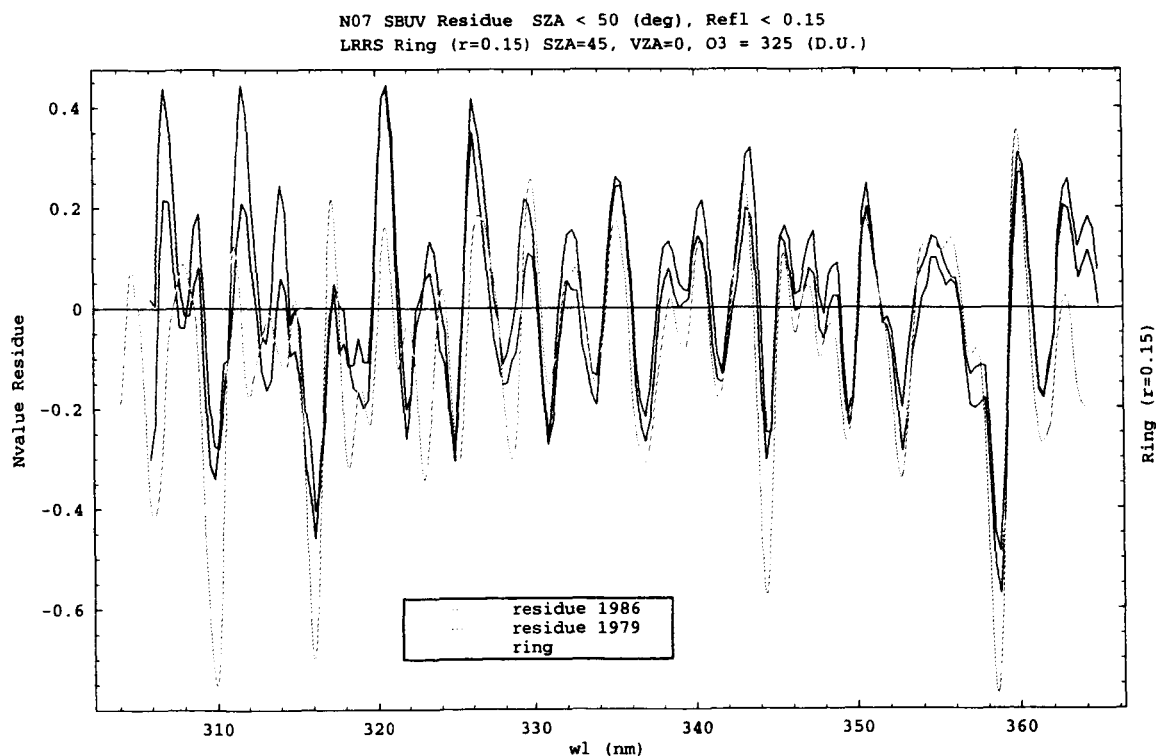
Results from this study confirm the data obtained from trial field measurements taken in August 2002 near Portland Oregon, as part of the NASA Sky DOAS Project. Inputs from this study were included in a successful proposal (G. Mount, PI) to develop more instrumentation for this project.

2 Report Summary Task 2

This task was done in collaboration with Kai Yang of SSAI. The motivation behind the work was to look at the average fitting residuals from the fitting of ozone total amounts from the sequence of continuous-scan SBUV measurements taken by Nimbus 7 from 1979 to 1986, and see to what extent these residuals are due to the Ring effect. Inelastic rotational Raman scattering was not considered in the forward model calculations involved in these fits.

The LIDORT-RRS model developed by the PI at SAO in 2002 was used to determine the Ring correction. LIDORT-RRS is a full discrete ordinate radiative transfer code which includes analytic solutions of first-order inelastic scattering due to rotational Raman transitions of O_2 and N_2 molecules. The wavelength range is from 310 to 360 nm. The Ring correction factor is here defined as the relative difference in the backscatter radiance calculated with and without the inclusion of the inelastic Raman source terms.

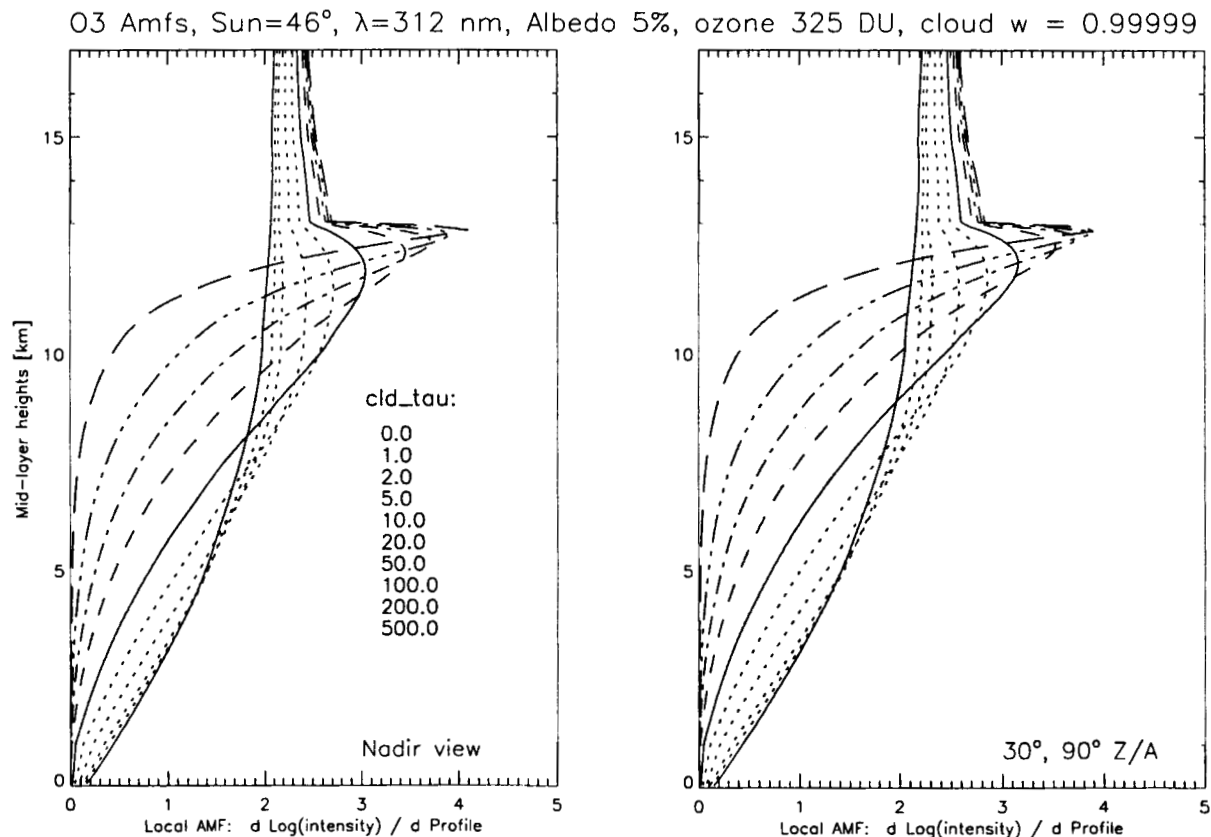
A sample is shown in Figure 3, where average 1979 and 1986 residuals for scenarios with solar zenith angles less than 50° and reflectivities less than 15% were compared with Ring correction factors computed with LIDORT-RRS for a solar zenith angle of 45° , total ozone column of 315 DU and for nadir viewing. It is clear that the Ring spectrum peaks and troughs follow the corresponding residual features closely, though the agreement is less good for wavelength below 323 nm.



3 Report Summary Task 3

This investigation looked at the enhanced sensitivity of backscatter radiances to ozone in the upper echelons of optically thick clouds in the troposphere. The background behind the study comes from a series of TOMS-based observations showing that for cloud-contaminated oceanic footprints, tropospheric ozone amounts in the Northern hemisphere are significantly larger than those observed in similar Southern hemisphere scenes. This has been attributed to ozone pollution in Northern hemisphere cloud fields. The underlying motivation is to develop a cloud slicing algorithm for tropospheric ozone without reference to surface albedo.

The study summarized below was started in Spring 2003, and is ongoing.



LIDORT Version 2.3E was used to generate analytic ozone profile weighting functions in a Rayleigh atmosphere with one or more cloud layers. Several cloud archetypes were considered, mainly confined to (1) nominal cloud between 4 and 6km, cirrus clouds between 11.5 and 12.5 km, fair weather cumulus clouds between 1 and 2 km, and deep convection clouds from 1 to 13 km. Calculations were performed at 2 wavelengths (312 and 320 nm), for 3 surface albedos (0.05, 0.5 and 0.95) for a solar zenith angle of 46 degrees. Most runs were done for cloud single scattering albedo of 0.99999,

though this quantity was adjusted downwards to look at the effect of particle absorption. Cloud optical thickness was allowed to vary from 1.0 to 500.0 depending on the cloud archetype. A mid-latitude ozone profile (from the TOMS Version 8 climatology) with total content 325 DU was chosen for the initial study.

To date, phase functions for all clouds except cirrus have been created using a set of 325 Legendre coefficients from a standard Mie calculation. In the LIDORT simulations, the single scatter contributions were calculated separately using the full phase function information (all 325 moments), while for the diffuse radiation field, the LIDORT multiple scatter calculations were done using 20 discrete ordinate streams in the half space, with the appropriate phase function truncation via the delta-M method. This was found to be accurate enough. For cirrus clouds, a set of Legendre coefficients at 550 nm was supplied by P. Yang (private communication) from one of the MODIS cloud algorithms.

Figure 4 is an example showing the enhancement effect for a deep convection cloud. Results for two viewing geometries are shown, with cloud optical thickness values as indicated. The weighting function profile is plotted as the derivative of the logarithm of backscatter radiance with respect to the layer partial column of ozone. This is equivalent to the definition of local-layer Air Mass Factors. The Rayleigh case (no cloud) is also shown for comparison.

Enhancement effects are relatively insensitive to choice of viewing geometry, but the presence of a bright surface enhances multiple scatter through middle and lower parts of the cloud layer, reducing somewhat the peak sensitivity, and also lowering the height at which the peak sensitivity occurs. Further tests have shown that the cloud sensitivity enhancement really picks up only for optically thick clouds (generally $\tau > 10$), and that the effect for cirrus and fair weather cumulus scenes is not significant. Further investigation will be confined mainly to deep-convection clouds.